

Magnetoresistance of $\text{YBa}_2\text{Cu}_3\text{O}_7$ in the “cold spots” model

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We calculate the in-plane magnetoresistance $\Delta\rho_{xx}/\rho_{xx}$ of $\text{YBa}_2\text{Cu}_3\text{O}_7$ in a magnetic field applied perpendicular to the CuO_2 planes for the “cold spots” model. In this model, the electron relaxation time $\tau_2 \propto 1/T^2$ at small regions on the Fermi surface near the Brillouin zone diagonals is much longer than the relaxation time $\tau_1 \propto 1/T$ at the rest of the Fermi surface (T is temperature). In qualitative agreement with the experiment, we find that Kohler’s rule is strongly violated, but the ratio $\Delta\rho_{xx}/\rho_{xx} \tan^2 \theta_H$, where $\tan \theta_H$ is the Hall angle, is approximately temperature-independent. We find the ratio is about 5.5, which is of the same order of magnitude as in the experiment.

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Theoretical interpretation of the electron transport properties in the normal state of high-temperature superconductors has attracted a great deal of attention (see references and discussion in Ref. [1]). In Ref. [1], we found that the frequency dependences of the longitudinal $\sigma_{xx}(\omega)$ and Hall $\sigma_{xy}(\omega)$ conductivities, measured in $\text{YBa}_2\text{Cu}_3\text{O}_7$ in Ref. [2], can be adequately fitted within a phenomenological model where different regions of the Fermi surface are characterized by two different relaxation times τ_1 and τ_2 . We called this model the additive two- τ model. We found that the electron relaxation time τ_2 at the “cold spots”, small regions on the Fermi surface near the Brillouin zone diagonals shown by the thick lines in Fig. 1, is much longer than the relaxation time τ_1 at the rest of the Fermi surface: $\tau_2/\tau_1 \approx 4$ at $T = 95$ K [1]. The microscopic origin of the cold spots is not very clear, but their pattern suggests that they may be related to the d -wave symmetry of the pseudogap in the normal state of cuprates [3]. In Ref. [1], we assumed for simplicity that the electron relaxation time changes discontinuously between the values τ_1 and τ_2 as a function of position on the Fermi surface. Recently, another version of the cold spots model was independently introduced by Ioffe and Millis [3]. In their model, the electron transport properties are completely determined by the cold spots, where the electron relaxation rate $1/\tau$ has a deep minimum:

$$1/\tau(k_t) - 1/\tau(\bar{k}_t) \propto (k_t - \bar{k}_t)^2. \quad (1)$$

In Eq. (1), k_t is the component of the electron wave vector tangential to the Fermi surface, which labels different points on the Fermi surface, and \bar{k}_t is its value at the center of a cold spot. Ioffe and Millis noticed that their model produces a magnetoresistance too high to agree with the experiment [4]. Magnetoresistance was discussed theoretically for the spinon-holon model in Ref. [4], for the charge-conjugation model in Ref. [5], and for the nearly-antiferromagnetic Fermi liquid model in Ref. [6]. In the present paper, we evaluate magnetoresistance for the additive two- τ model of Ref. [1]. (See also a comment on this model in Ref. [7].)

The high-temperature cuprate superconductors can be modeled as two-dimensional (2D) square lattices parallel

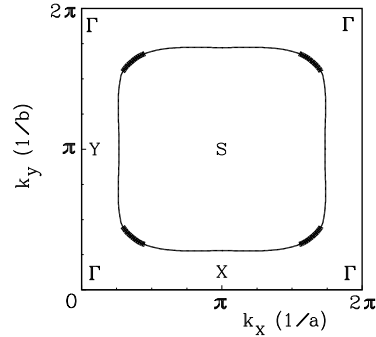


FIG. 1. Fermi surface of the CuO_2 bonding band of $\text{YBa}_2\text{Cu}_3\text{O}_7$ according to the band-structure calculations [8]. The thick lines indicate the “cold spots”.

to the (x, y) plane and spaced with the distance d along the z axis. We consider the case where a weak magnetic field H is applied perpendicular to the planes and study the in-plane transport properties. For this purpose, we may neglect coupling between the layers and consider the 2D electron wave vector \mathbf{k} and energy $\varepsilon(\mathbf{k})$. The linearized stationary Boltzmann equation [9], written for the deviation $\chi(\mathbf{k})$ of the electron distribution function $f(\mathbf{k})$ from the equilibrium Fermi function $f_0(\varepsilon)$: $f(\mathbf{k}) - f_0(\varepsilon) = -\chi(\mathbf{k}) \partial f_0(\varepsilon)/\partial \varepsilon$, has the form:

$$\frac{eH}{\hbar c} l(k_t) \frac{d\chi(k_t)}{dk_t} + \chi(k_t) = e\mathbf{E} \cdot \mathbf{l}(k_t), \quad (2)$$

where $\mathbf{l}(k_t) = \mathbf{v}(k_t)\tau(k_t)$ and $\mathbf{v}(k_t) = \partial \varepsilon(\mathbf{k})/\hbar \partial \mathbf{k}$ are the local values of the electron mean-free path and velocity at a point k_t on the Fermi surface. (e is the electron charge, \hbar is Planck’s constant, and c is the speed of light.)

In the case of a weak magnetic field H , the first term in Eq. (2) is a small perturbation, so a solution can be obtained as the Jones-Zener series in powers of H by iterating this term:

$$\chi(k_t) = e \sum_{n=0}^{\infty} \left(-\frac{eH}{\hbar c} l(k_t) \frac{d}{dk_t} \right)^n \mathbf{E} \cdot \mathbf{l}(k_t). \quad (3)$$

Using Eq. (3), we calculate the electric current $\mathbf{j} = 2e \sum_{\mathbf{k}} \mathbf{v}(\mathbf{k}) f(\mathbf{k})$, where the coefficient 2 accounts for two spin orientations of electrons, and find the conductivity tensor:

$$\sigma_{ij} = \frac{2e^2}{(2\pi)^2 \hbar d} \sum_{n=0}^{\infty} \oint dk_t \frac{l_i(k_t)}{l(k_t)} \left(-\frac{eH}{\hbar c} l(k_t) \frac{d}{dk_t} \right)^n l_j(k_t).$$

Here the integral in k_t is taken around the Fermi surface. For a system of tetragonal symmetry, the diagonal conductivity $\sigma_{xx} = \sigma_{xx}^{(0)} + \sigma_{xx}^{(2)}$ up to the second order in H and the Hall conductivity σ_{xy} linear in H are given by the following expressions [10,4]:

$$\sigma_{xx}^{(0)} = \frac{e^2}{(2\pi)^2 \hbar d} \oint dk_t l(k_t), \quad (4)$$

$$\sigma_{xy} = \frac{e^3 H}{(2\pi)^2 \hbar^2 c d} \oint \mathbf{e}_z \cdot [\mathbf{l}(k_t) \times d\mathbf{l}(k_t)], \quad (5)$$

$$\begin{aligned} \sigma_{xx}^{(2)} &= \frac{2e^4 H^2}{(2\pi)^2 \hbar^3 c^2 d} \oint dk_t l_x(k_t) \frac{d}{dk_t} \left(l(k_t) \frac{dl_x(k_t)}{dk_t} \right), \\ &= -\frac{2e^4 H^2}{(2\pi)^2 \hbar^3 c^2 d} \oint dk_t l(k_t) \left(\frac{dl_x(k_t)}{dk_t} \right)^2, \end{aligned} \quad (6)$$

where \mathbf{e}_z is a unit vector along the z axis. According to Eq. (6), magnetic field always reduces the conductivity: $\sigma_{xx}^{(2)} < 0$.

When evaluated for a discontinuous function $\tau(k_t)$, Eqs. (4) and (5) give finite results, which were studied in Ref. [1]. However, Eq. (6) gives an infinite value for $\sigma_{xx}^{(2)}$ because of the squared derivative $[d\tau(k_t)/dk_t]^2$ of a discontinuous function $\tau(k_t)$. In order to obtain a finite result, we introduce a smooth interpolation between the two values of τ in a transition interval of the width κ :

$$\tau(k_t) = \frac{\tau_1 + \tau_2}{2} \mp \frac{\tau_1 - \tau_2}{2} \tanh \left(\frac{k_t - \tilde{k}_t}{\kappa} \right), \quad (7)$$

where \tilde{k}_t is the boundary between the “hot” and “cold” regions. We find the following three contributions to $\sigma_{xx}^{(2)}$:

$$\sigma_{xx}^{(2)} = -C_1 \tau_1^3 - C_2 \tau_2^3 - \tilde{\sigma}_{xx}^{(2)}. \quad (8)$$

The coefficients C_1 and C_2 are given by the integrals over the “hot” and “cold” regions of the Fermi surface, where the relaxation times are τ_1 and τ_2 , respectively:

$$C_{1,2} = \frac{2e^4 H^2}{(2\pi)^2 \hbar^3 c^2 d} \int_{1,2} dk_t v(k_t) \left(\frac{dv_x(k_t)}{dk_t} \right)^2. \quad (9)$$

The first two terms in Eq. (9) do not depend on κ . The last term in Eq. (8) comes from the transition interval between the “hot” and “cold” areas:

$$\tilde{\sigma}_{xx}^{(2)} = \frac{2e^4 H^2}{(2\pi)^2 \hbar^3 c^2 d} v^3(\tilde{k}_t) \frac{(\tau_1 + \tau_2)(\tau_1 - \tau_2)^2}{6\kappa}. \quad (10)$$

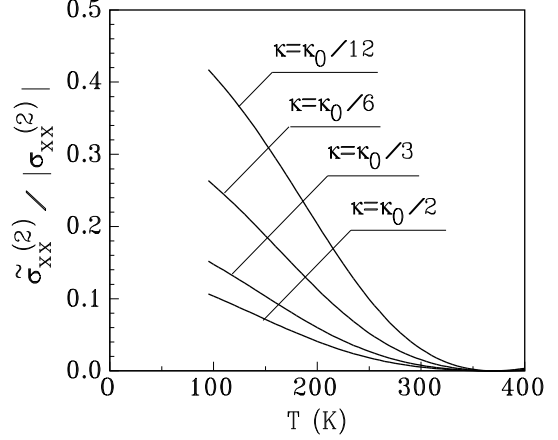


FIG. 2. Contribution of the transitory zone between the “hot” and “cold” regions on the Fermi surface to magnetoconductivity, $\tilde{\sigma}_{xx}^{(2)}$, normalized to the total magnetoconductivity $|\sigma_{xx}^{(2)}|$ and shown as a function of temperature. Different curves correspond to different sizes of the transition interval κ , indicated as a fraction of the size κ_0 of a “cold spot”.

This term becomes singular when the width of the transition interval is reduced to zero: $\tilde{\sigma}_{xx}^{(2)} \rightarrow \infty$ when $\kappa \rightarrow 0$.

Using Eqs. (8), (9), and (10) with the parameters determined in Ref. [1], we calculate $\sigma_{xx}^{(2)}$ for the CuO_2 bonding band of $\text{YBa}_2\text{Cu}_3\text{O}_7$ shown in Fig. 1. As in Ref. [1], we neglect contributions of the other bands. We phenomenologically assign linear and quadratic temperature dependences to the scattering rates in the “hot” and “cold” regions:

$$\tau_1^{-1} \propto T, \quad \tau_2^{-1} \propto T^2, \quad (11)$$

with the same parameters as Ref. [1]. Computing the integrals (9) over the Fermi surface, we find that the ratio $C_1 : C_2$ turns out to be the same as the ratio $b_1 : b_2 = 0.71 : 0.29$ in Ref. [1].

The size of the transition interval, κ , is limited from above by the size $\kappa_0 = 0.6/a$ of a cold spot: $\kappa \leq \kappa_0$, where a is the CuO_2 lattice spacing. In Fig. 2, we show the ratio $\tilde{\sigma}_{xx}^{(2)} / |\sigma_{xx}^{(2)}|$ computed for different values of κ . We observe that $\tilde{\sigma}_{xx}^{(2)}$ produces a significant contribution to $\sigma_{xx}^{(2)}$ only when the transition interval becomes very small: $\kappa \leq \kappa_0/12$. For a realistic width, $\kappa = \kappa_0/2$, the contribution of the transition interval is insignificant: $\tilde{\sigma}_{xx}^{(2)} \ll |\sigma_{xx}^{(2)}|$.

The experimentally measurable quantity is the magnetoresistance $\Delta\rho_{xx} = \rho_{xx}(H, T) - \rho_{xx}(0, T)$, which is related to the conductivities by the formula

$$\Delta\rho_{xx}/\rho_{xx} = -\sigma_{xx}^{(2)}/\sigma_{xx}^{(0)} - \tan^2 \theta_H, \quad (12)$$

where $\tan \theta_H = \sigma_{xy}/\sigma_{xx}^{(0)}$ is the Hall angle. Fig. 3 shows the calculated temperature dependence of magnetoresistance $\Delta\rho_{xx}/\rho_{xx}$ at $H = 9$ T for different values of κ .

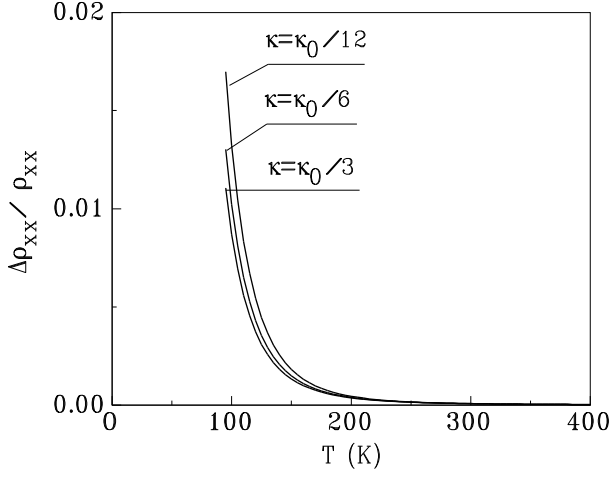


FIG. 3. Magnetoresistance $\Delta\rho_{xx}/\rho_{xx}$ as a function of temperature in the magnetic field $H = 9$ T.

It is more convenient to study the dimensionless ratio

$$\zeta = \Delta\rho_{xx}/\rho_{xx} \tan^2 \theta_H = -\sigma_{xx}^{(2)}\sigma_{xx}^{(0)}/\sigma_{xy}^2 - 1, \quad (13)$$

which does not depend on magnetic field. In the Drude model with a single relaxation time $\tau(T)$, ζ does not depend on temperature, because $\tau(T)$ cancels out, and is equal to

$$\bar{\zeta} = \frac{\oint dk_t v(k_t) (dv_x(k_t)/dk_t)^2 \oint dk_t v(k_t)}{2(\oint dk_t v_x(k_t) dv_y(k_t)/dk_t)^2} - 1. \quad (14)$$

It was found experimentally that ζ is nearly temperature-independent and equals $1.5 \div 1.7$ in $\text{YBa}_2\text{Cu}_3\text{O}_7$, 13.6 in $\text{La}_2\text{Sr}_x\text{CuO}_4$ [4], 3.6 in optimally doped and 2.0 in over-doped $\text{Tl}_2\text{Ba}_2\text{CuO}_{6+\delta}$ [5,11]. These results are quite remarkable given that electron transport in cuprates *cannot* be described by a single-relaxation-time Drude model. In the spinon-holon model of Ref. [4], ζ is given by the same temperature-independent expression (14) as in the simple Drude model, because the two relaxation times τ_{tr} and τ_H cancel out.

In Fig. 4, we plot $\zeta(T)$ calculated using Eqs. (8)–(13) for different values of κ . For a realistic $\kappa = \kappa_0/2$, we observe that ζ is approximately temperature-independent. This is quite surprising considering that $\zeta(T)$ is given by a complicated rational function of temperature. This result demonstrates that, contrary to the conclusion made in Ref. [4], ζ can be temperature-independent in a Fermi-liquid model [1,12,13], where different regions on the Fermi surface have different temperature dependences of τ given by Eq. (11). We wish to emphasize that we do not optimize the parameters of the model to make ζ temperature-independent; we use the same parameters that have been found already in Ref. [1] by fitting frequency dependences of σ_{xx} and σ_{xy} . As Fig. 4 shows, the value of ζ is about 5.5 , which is close to the Drude value $\bar{\zeta} = 5.67$ calculated from Eq. (14) for the Fermi

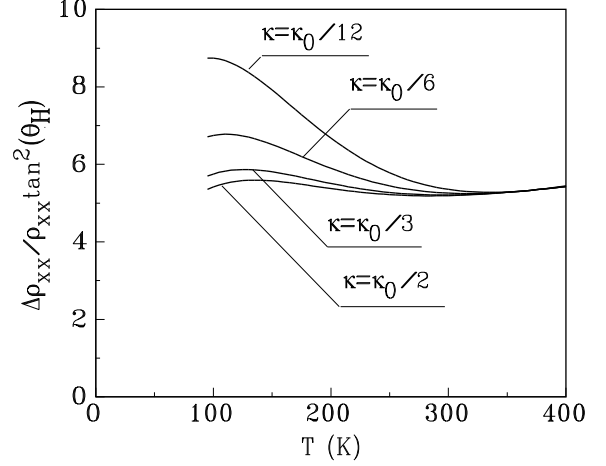


FIG. 4. Dimensionless ratio of magnetoresistance and the Hall angle squared, $\Delta\rho_{xx}/\rho_{xx} \tan^2 \theta_H$, as a function of temperature for different values of κ .

surface shown in Fig. 1. While the theoretical value of ζ is greater than the experimental one in $\text{YBa}_2\text{Cu}_3\text{O}_7$ by a factor of 3, both values are of the same order of magnitude. The discrepancy could be ascribed to an excessive flatness of our model Fermi surface compared with the real one, which reduces $\tan^2 \theta_H$ and increases ζ . This suggestion is supported by the fact that the highest value of ζ is found in $\text{La}_2\text{Sr}_x\text{CuO}_4$, where the Fermi surface is believed to be the flattest. (Eq. (14) gives zero for a circular Fermi surface.)

Because ζ is approximately temperature-independent, and our model gives approximately $\tan \theta_H \propto 1/T^2$ and $\rho_{xx} \propto T$ [1], we conclude that $\Delta\rho_{xx}/\rho_{xx} \propto 1/T^4$, in agreement with the experiment [4]. Kohler's rule, which states that, in a single-relaxation-time model, $\Delta\rho_{xx}(H, T)/\rho_{xx}(0, T)$ is a function of $H/\rho_{xx}(0, T)$, is strongly violated in cuprates [4]. In a weak magnetic field, where $\Delta\rho_{xx}/\rho_{xx} \propto H^2$, Kohler's rule requires that $\Delta\rho_{xx}(H, T)\rho_{xx}(0, T)$ should not depend on temperature. In Fig. 5, we show $\Delta\rho_{xx}(H, T)\rho_{xx}(0, T)$ normalized to $\rho_{xx}^2(0, T = 95 \text{ K})$ as a function of temperature for different values of κ at $H = 9$ T. We observe a strong temperature dependence $\Delta\rho_{xx}\rho_{xx} \propto 1/T^2$, which demonstrates that Kohler's rule is violated in our model because of the different temperature dependences of τ_1 and τ_2 in Eq. (11).

We now briefly compare the cold spots models of Refs. [1] and [3]. In the latter model, transport properties are determined by the relaxation time at the center of a cold spot, $\tau(\vec{k}_t)$, denoted as τ_{FL} in Ref. [3] and roughly corresponding to our τ_2 . The second relaxation time τ_1 does not appear explicitly in the model [3], so only one relaxation time τ_{FL} controls frequency dependence of transport properties. The expression for diagonal conductivity in the model [3],

$$\sigma_{xx}(\omega) \propto 1/\sqrt{1 - i\omega\tau_{\text{FL}}}, \quad (15)$$

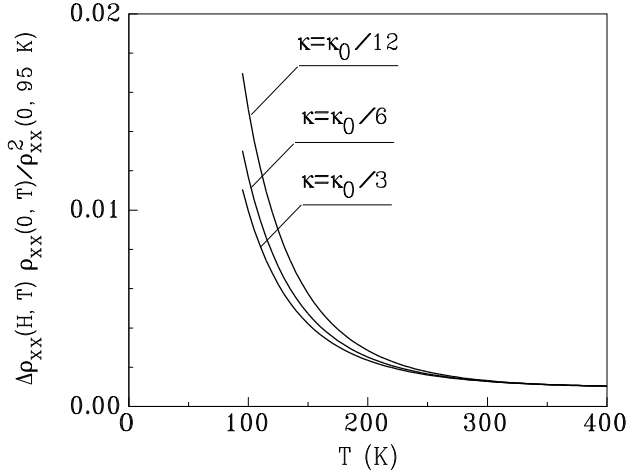


FIG. 5. The combination $\Delta\rho_{xx}(H, T)\rho_{xx}(0, T)/\rho_{xx}^2(0, 95 \text{ K})$ that would be temperature-independent if Kohler's rule were satisfied. The curves are calculated for the magnetic field $H = 9 \text{ T}$.

fits the experimental data of Ref. [14] at $T = 200 \text{ K}$. The expression for the Hall cotangent in the model [3],

$$\cot \theta_H(\omega) \propto 1 - i\omega\tau_{\text{FL}}, \quad (16)$$

fits the experimental data of Ref. [2] at $T = 95 \text{ K}$ with $1/\tau_{\text{FL}} = 54 \text{ cm}^{-1} = 7 \text{ meV}$ [1]. Substituting this value of $1/\tau_{\text{FL}}$ into Eq. (15), we calculate $\sigma_{xx}(\omega)$ and show the result in Fig. 6. In this figure, the solid line with squares represents frequency dependence of transmittance through a thin film of $\text{YBa}_2\text{Cu}_3\text{O}_7$ (which is determined by $\sigma_{xx}(\omega)$) for the model [3]. Dots represent the experimental data of Ref. [2]; the solid and dashed lines show fits for the additive and multiplicative two- τ models studied in Ref. [1]. The overall coefficient in Eq. (15) has been selected to fit the experimental value at $\omega = 0$. We observe that the curve for the model [3] does not match the experimental data of Ref. [2]. The reason for this failure is that fitting both $\sigma_{xx}(\omega)$ and $\sigma_{xy}(\omega)$ requires two different frequency scales, such as $1/\tau_1$ and $1/\tau_2$ [1], whereas the model [3] has only one frequency scale $1/\tau_{\text{FL}}$.

In conclusion, we have calculated the in-plane magnetoresistance $\Delta\rho_{xx}/\rho_{xx}$ of $\text{YBa}_2\text{Cu}_3\text{O}_7$ in a magnetic field applied perpendicular to the CuO_2 planes for the additive two- τ model of Ref. [1]. We find that Kohler's rule is strongly violated, but the ratio $\Delta\rho_{xx}/\rho_{xx} \tan^2 \theta_H$ is approximately temperature-independent and, for the model Fermi surface employed, is approximately equal to 5.5. The theoretical results agree qualitatively and, within an order of magnitude, quantitatively with the experiment.

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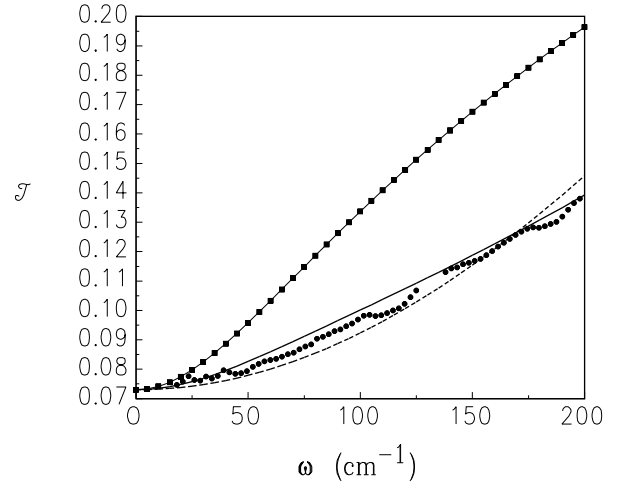


FIG. 6. Frequency dependence of the transmittance $T(\omega)$ through a thin film of $\text{YBa}_2\text{Cu}_3\text{O}_7$ in zero magnetic field. Dots: experimental data from Ref. [2]; solid and dashed lines: fits to the additive and multiplicative two- τ models of Ref. [1]; solid line with squares: calculation for the cold spots model of Ref. [3].

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